



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



# **IMPACT-Z and IMPACT-T: Code Improvements and Applications**

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# IMPACT: A 3D Parallel Beam Dynamics Code Suite

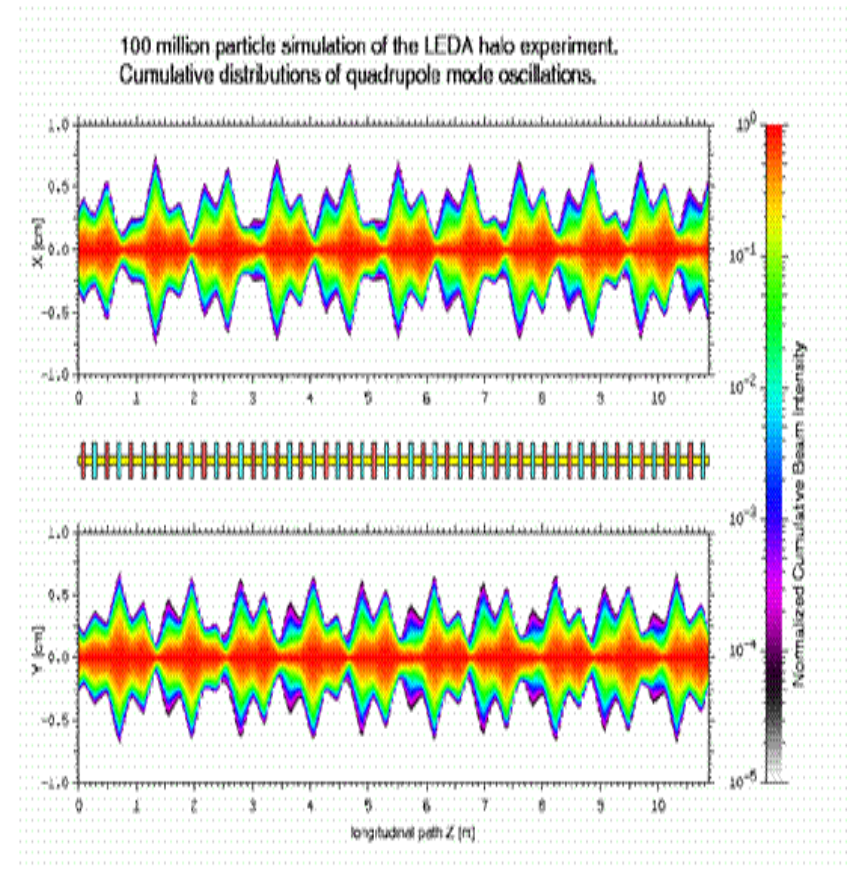


- IMPACT-Z
  - Parallel particle-in-cell (PIC) code used for electron & ion linacs
- IMPACT-T
  - Parallel PIC code used for photoinjectors
- Fix3D/2D
  - RMS envelope code for match and analysis
- Pre and Post-Processing
  - Matlab script for parameter optimization with IMPACT code
  - Python script for initial driven phase setting
  - Fourier coefficients calculation field
  - Slice emittances, uncorrelated energy spread

# IMPACT-Z



- Parallel PIC code using coordinate “z” as the independent variable
- Key Features
  - Detailed RF accelerating and focusing model
  - Multiple 3D Poisson solvers
    - Variety of boundary conditions
    - 3D Integrated Green Function
  - Multi-charge state
  - Machine error studies and steering
  - Wakes
  - CSR (1D)
  - Run on both serial and multiple processor computers



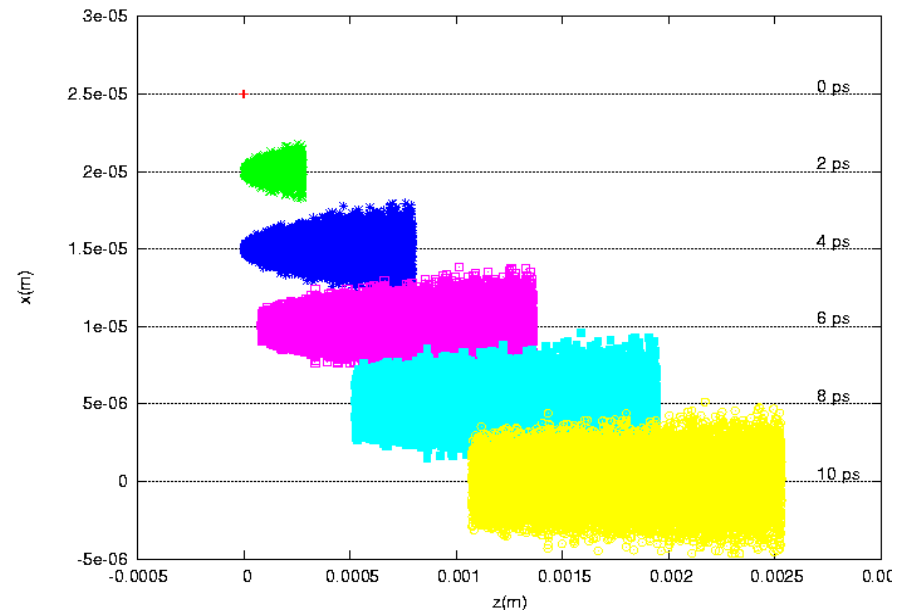
# IMPACT-T



- Parallel PIC code using time “t” as the independent variable

- Key Features

- Detailed RF accelerating and focusing model
- Multiple Poisson solvers
  - 3D Integrated Green Function
  - point-to-point
- Multiple species
- Monte Carlo gas ionization model (in progress)
- Cathode image effects
- Wakes
- CSR (1D)
- Run on both serial and multiple processor computers



Emission from nano-needle tip  
including Borsch effect

# IMPACT-Z: Code Improvements (cont'd)



- Defects fixing
  - ✓ In Lorentz integrator
  - ✓ z-to-t transfer for multiple charge state
  - ✓ linear transfer map for hard edge quadrupole
  - ✓ charge state update
- External map getting for all particles at one location for DTL and CCL modules
- Quiet start for an initial particle sampling
- Multiple reference particle for SolRF and TWS modules
- A new upsampling scheme
- Code improvement for 5 billion particle simulation
- 1D CSR wake field including transition
- Two RF/DC discrete fields overlap in one beam line element

# IMPACT-Z: Code Improvements



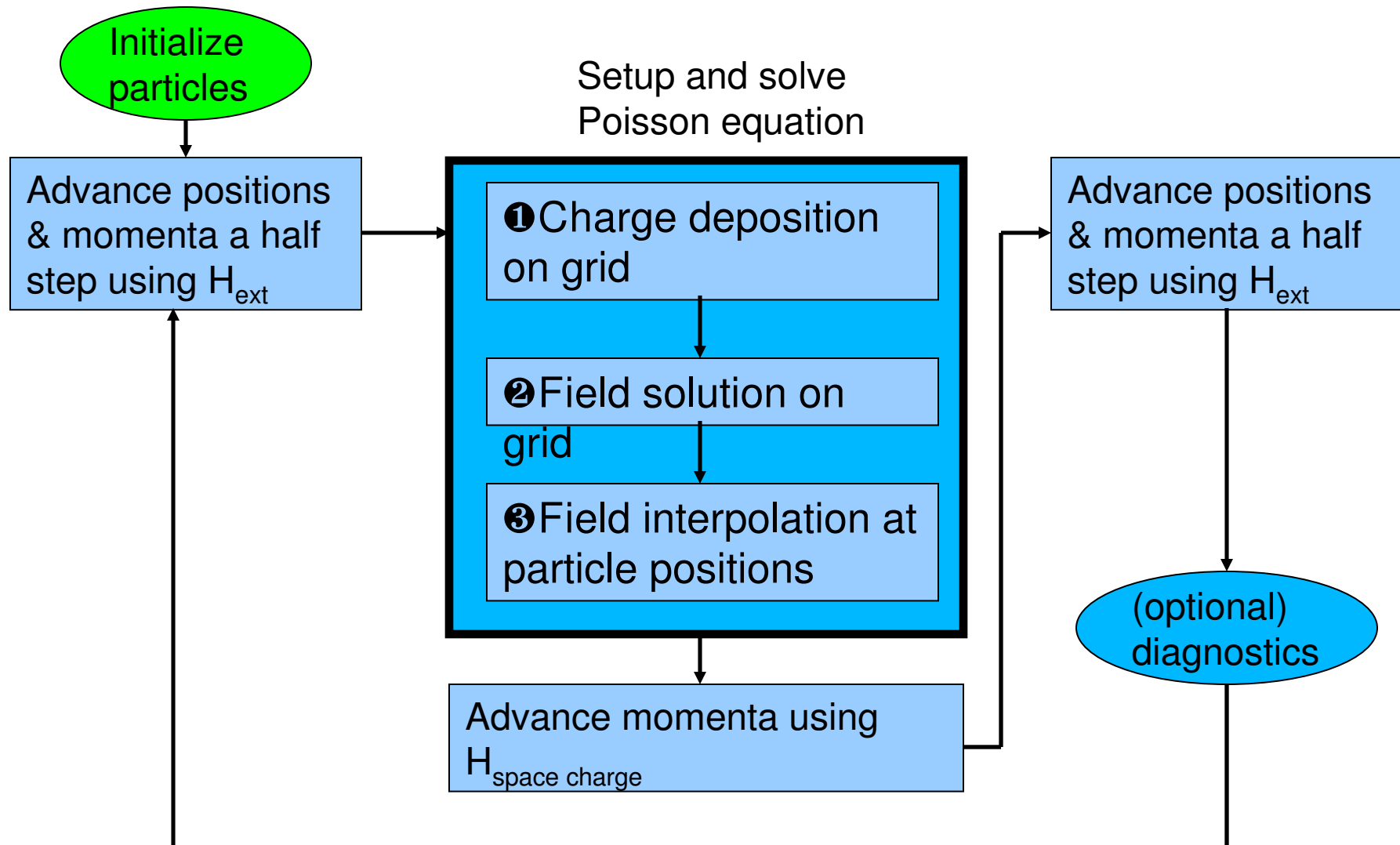
- Multipole element: quadrupole – dodecapole
- FFTw option for open boundary field solver
- Instant phase rotation
- Python script utilities
  - ✓ Convert MAD input lattice into IMPACT input lattice
  - ✓ Convert Elegant input lattice into IMPACT input lattice (in progress)
  - ✓ Convert Parmila input lattice into IMPACT input lattice (in progress)
  - ✓ Set up initial driven phase along the beam line
  - ✓ Integrate IMPACT and GANT linac collimator module
  - ✓ Automatic multiple plot output (in progress)
  - ✓ Multiple charge beam steering capability
- Matlab script utilities
  - ✓ Integrate the IMPACT beam dynamics simulation with parameter optimization scheme

# IMPACT-T: Code Improvements



- Defects fixing
  - ✓ sampling semi-Gaussian distribution
- Quiet start for initial particle sampling
- Multiple slice longitudinal Gaussian distribution
- 1<sup>st</sup> order particle emission model
- Longitudinal random computational box resizing
- Mechanic momentum -> canonical momentum in solenoid
- Parallel particle-field decomposition
- Snapshot output of rms information of the beam
- Snapshot output of slice information of the beam
- Discrete external field read in for SolRF element
- Skew quadrupole

# Particle-In-Cell Simulation with Split-Operator Method



# Green Function Solution of Poisson's Equation (with 3D Open Boundary Conditions)



$$\phi(r) = \int G(r, r') \rho(r') dr'$$
$$\phi(r_i) = h \sum_{i'=1}^N G(r_i - r_{i'}) \rho(r_{i'})$$

$$G(x, y, z) = 1 / \sqrt{(x^2 + y^2 + z^2)}$$

Direct summation of the convolution scales as  $N^6$  !!!!  
N – grid number in each dimension

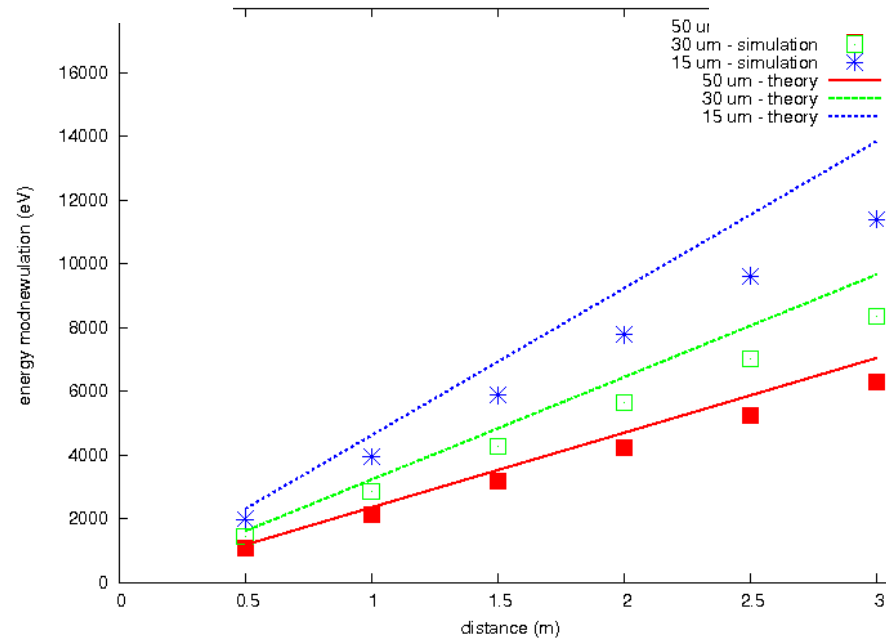
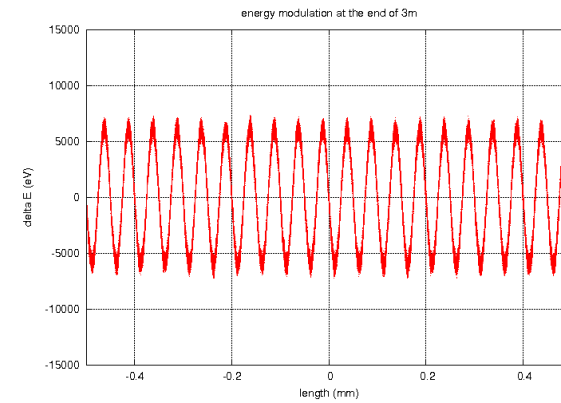
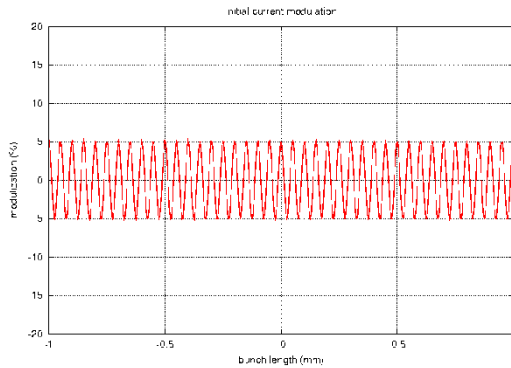
Hockney's Algorithm:- *scales as  $(2N)^3 \log(2N)$*

- Ref: Hockney and Easwood, *Computer Simulation using Particles*, McGraw-Hill Book Company, New York, 1985.

$$\phi_c(r_i) = h \sum_{i'=1}^{2N} G_c(r_i - r_{i'}) \rho_c(r_{i'})$$

$$\phi(r_i) = \phi_c(r_i) \quad \text{for } i = 1, N$$

# Space-Charge Driven Energy Modulation vs. Distance in a Drift Space



$$F_x(s) = q \int_{-\infty}^{+\infty} W_T(s-s') x(s') \lambda(s') ds'$$

$$F_z(s) = \int_{-\infty}^{+\infty} W_L(s-s') \lambda(s') ds'$$

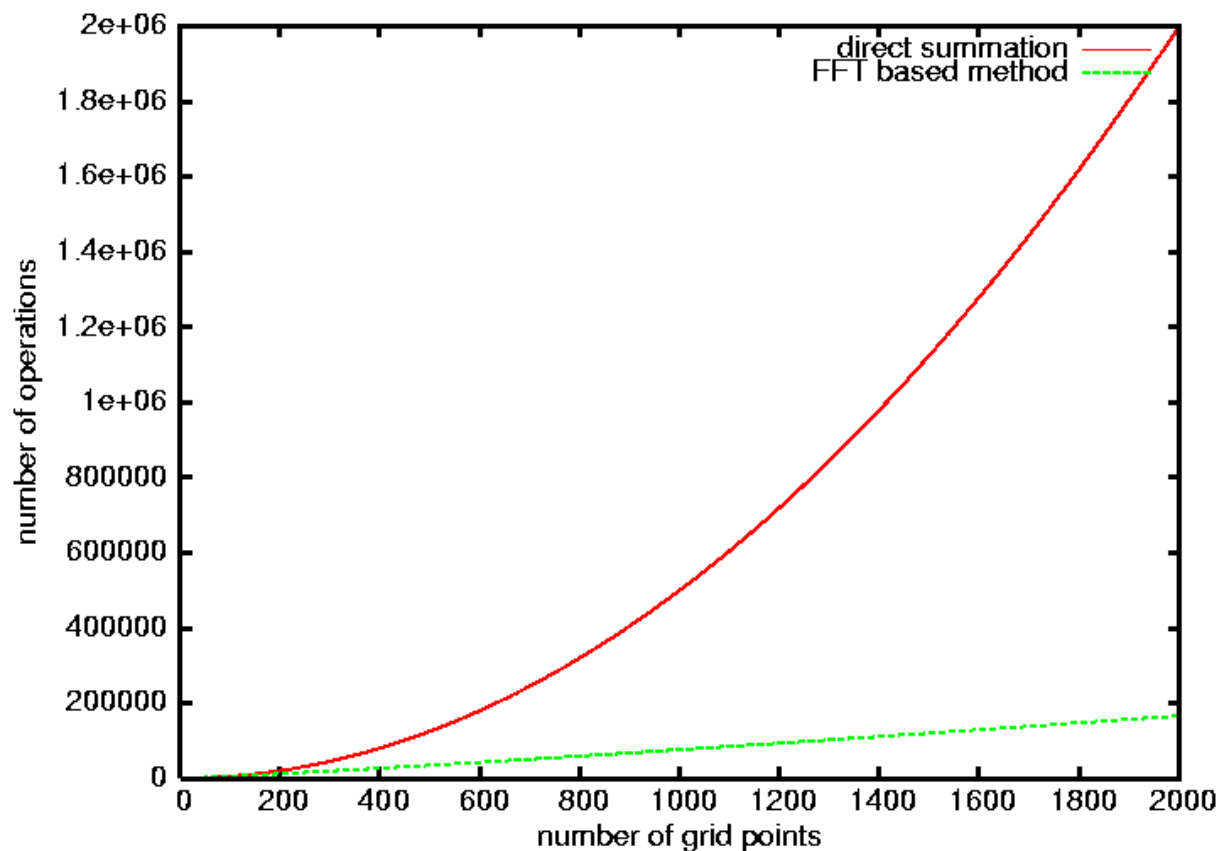
$$F(s) = \int_{-\infty}^{+\infty} G(s-s') \rho(s') ds'$$

$$G(s) = \begin{cases} W(s) & \text{for } s \geq 0 \\ 0 & \text{for } s < 0 \end{cases}$$

$$F_c(s_i) = h \sum_{i'=1}^{2N} G_c(s_i - s_{i'}) \rho_c(s_{i'})$$

$$F(s_i) = F_c(s_i) \quad \text{for } i = 1, \dots, N$$

# Computing Operation Comparison between the Direct Summation and the FFT Based Method



# 1D CSR Wake Field Including Transient Effects



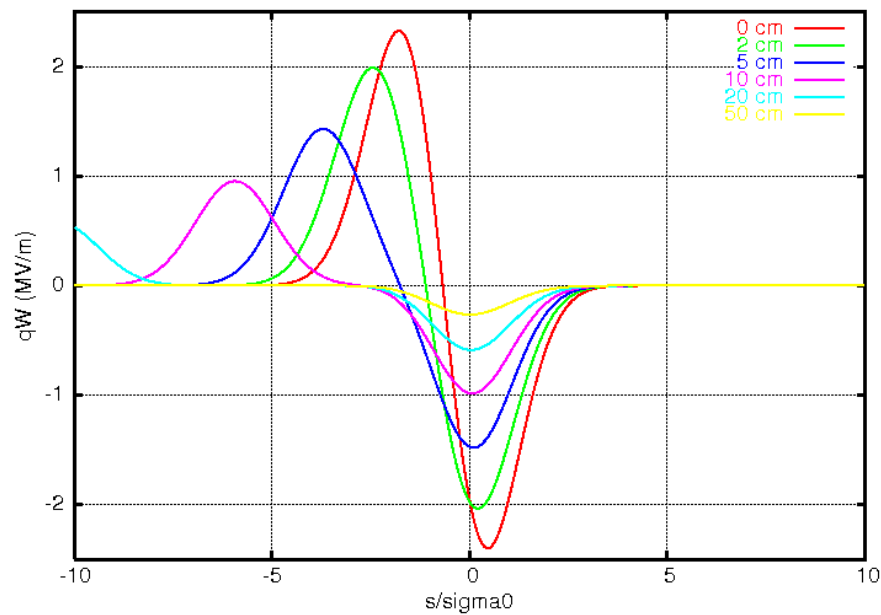
$$\frac{dE(s, \phi)}{cdt} = -\frac{2e^2}{4\pi\epsilon_0 3^{1/3} R^{2/3}} \left( \int_{s-s_L}^s \frac{1}{(s-s')^{1/3}} \frac{\partial \lambda(s')}{\partial s'} ds' + \frac{\lambda(s-s_L) - \lambda(s-4s_L)}{s_L^{1/3}} \right)$$

$$W(s) = \begin{cases} -\frac{4}{R} \frac{1}{(\phi_m + 2x)} \lambda\left(s - \frac{R}{6} \phi_m^2 (\phi_m + 3x)\right) & \text{for source in front of the bend} \\ \frac{4}{R} \left( \frac{\lambda(s - \Delta s_{max})}{(\phi_m + 2x)} + \int_{s - \Delta s_{max}}^s \frac{1}{\psi + 2x} \frac{\partial \lambda}{\partial s'} ds' \right) & \text{for source inside the bend} \end{cases}$$

$$s - s' = \frac{R\psi^3}{24} \frac{\psi + 4x}{\psi + x}$$

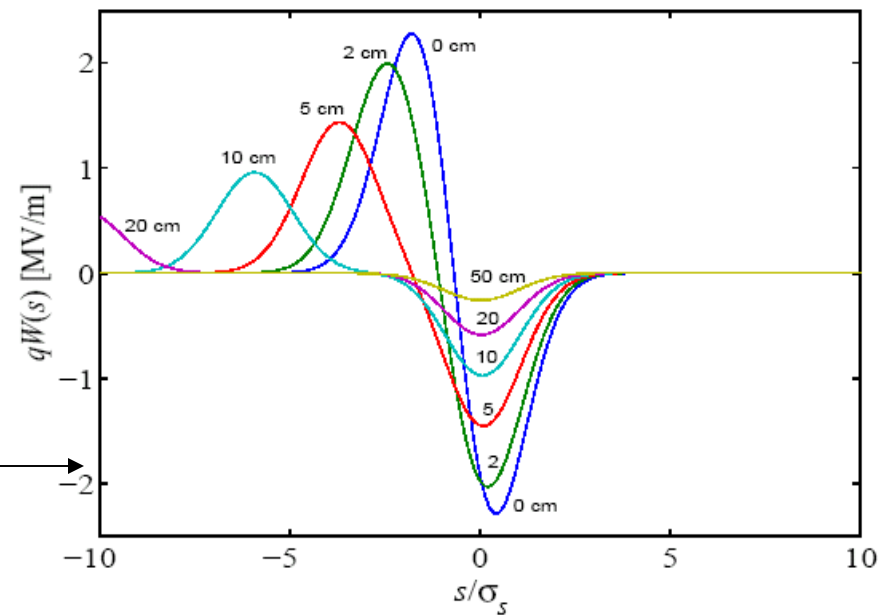
Ref: 1) E. L. Saldin, E. A. Schneidmiller, and M. V. Yurkov,  
Nucl. Instrum. Methods Phys. Res., Sect. A398, 373 (1997).  
2) M. Borland, Phys. Rev. Sepecial Topics - Accel. Beams 4, 070701 (2001).  
3) G. Stupakov and P. Emma, ``CSR Wake for a Short Magnet in Ultrarelativistic Limit,"  
SLAC-PUB-9242, 2002.

# Test of the CSR Wake Implementation for a Short Bend

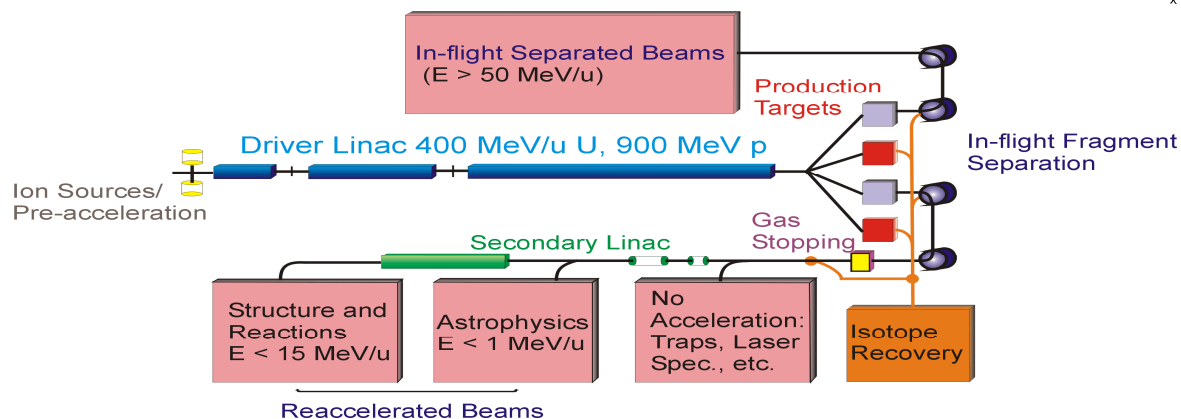
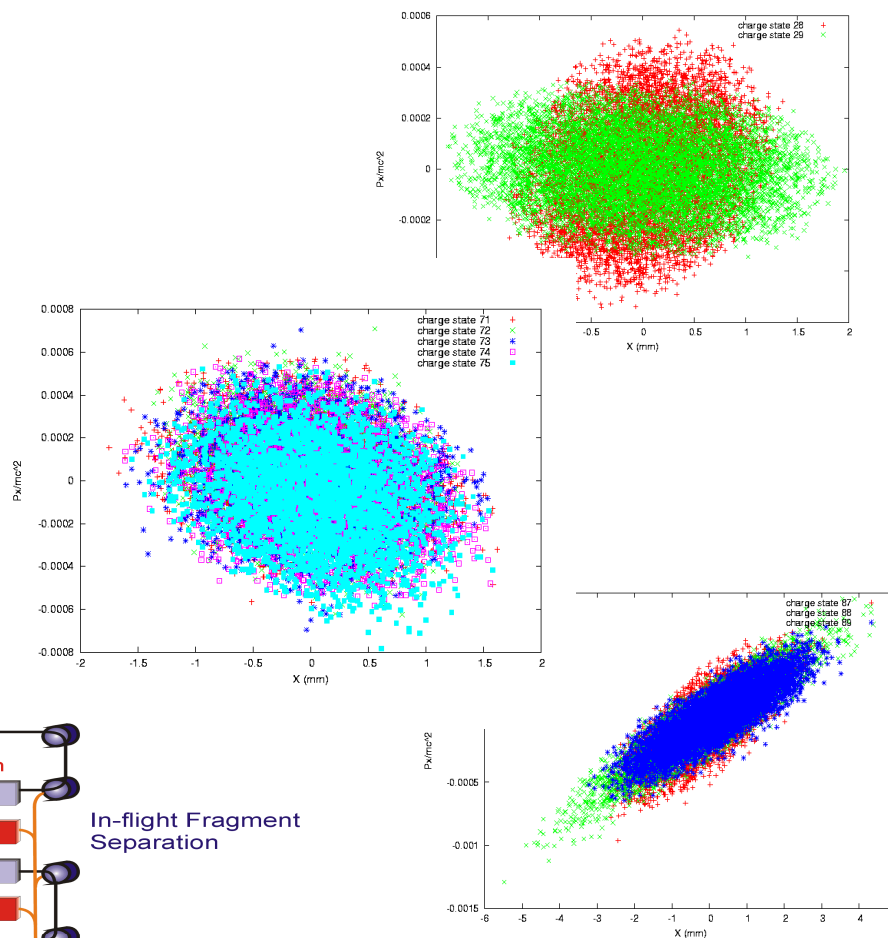
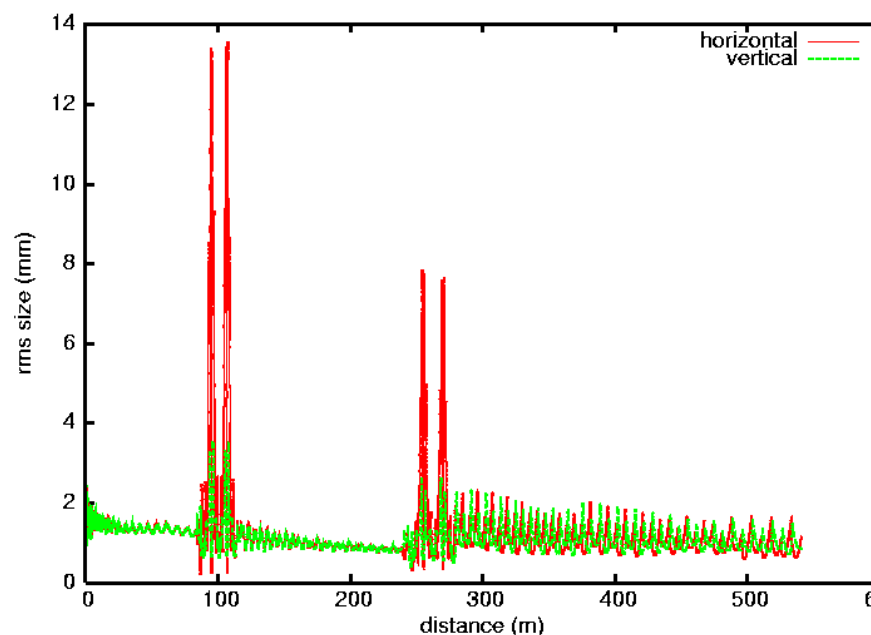


$R = 1.5$  m, Arc=10 cm

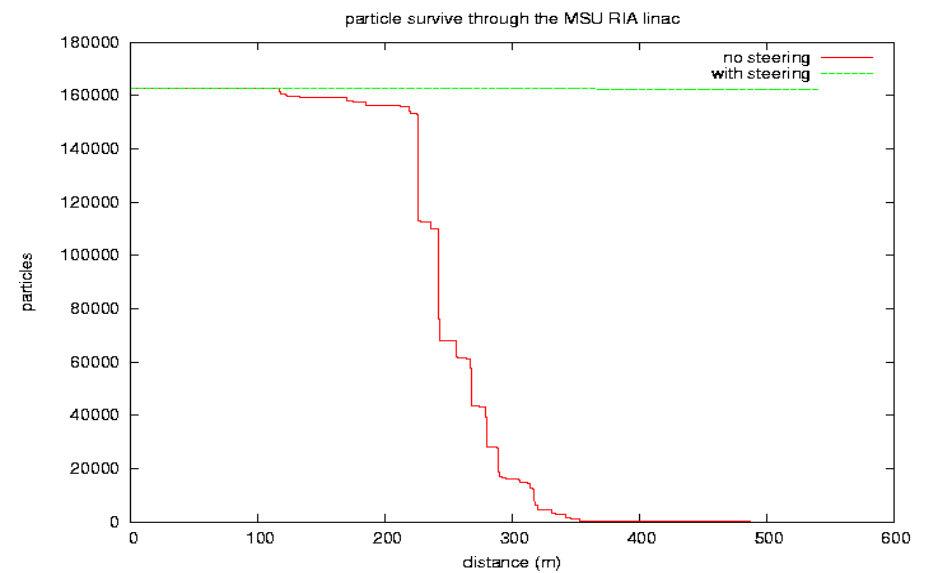
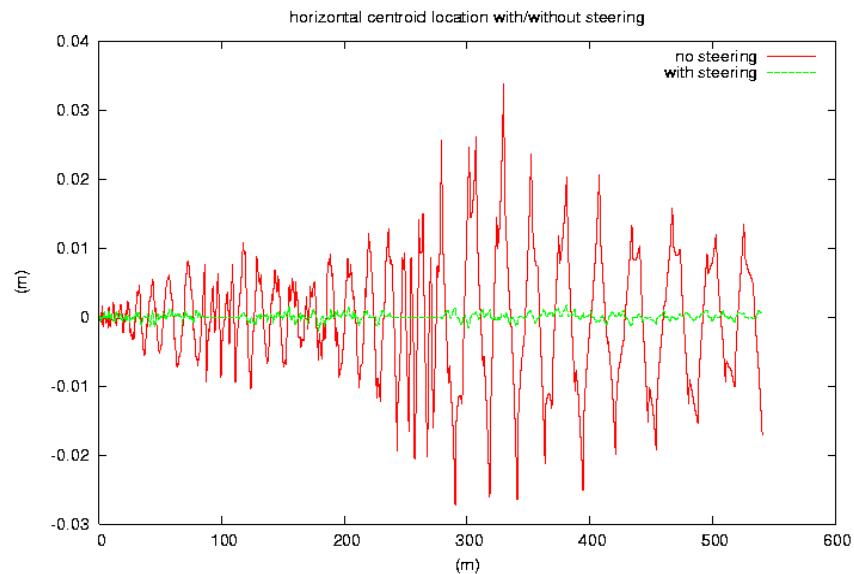
From G. Stupakov and P. Emma



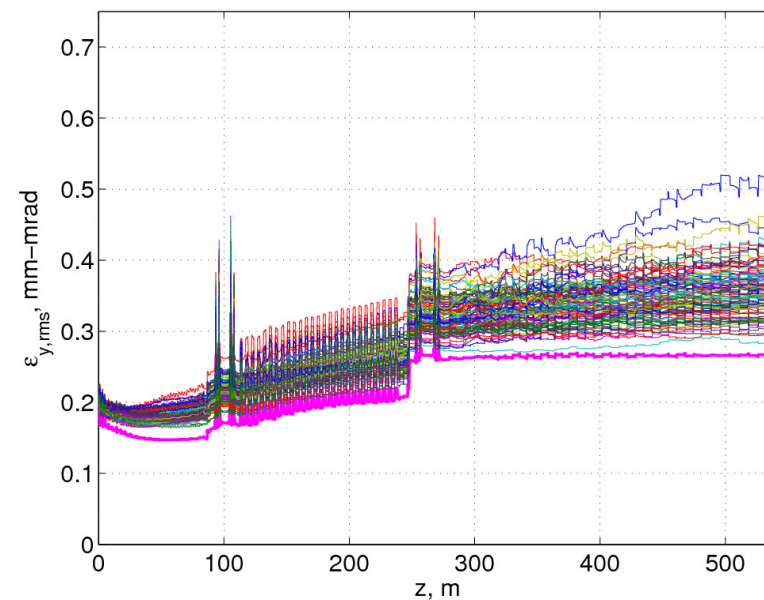
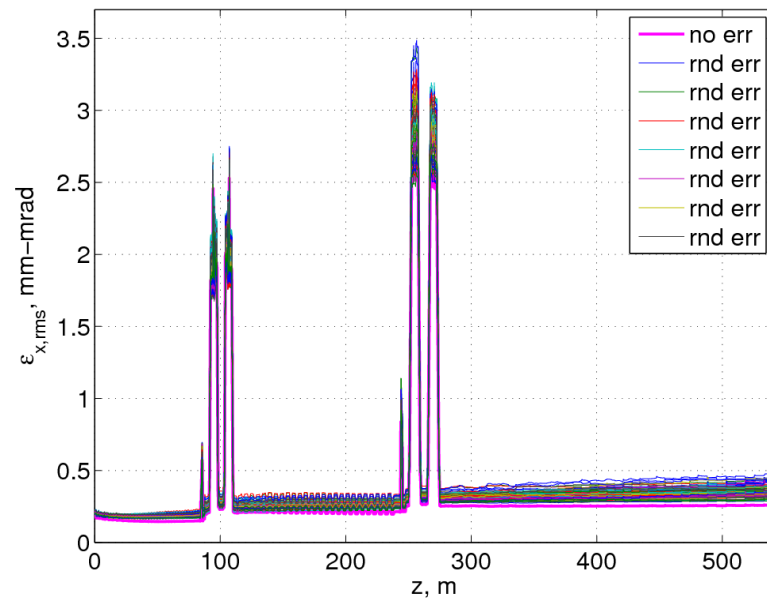
# IMPACT-Z multi-charge-state simulation of beam dynamics in proposed MSU RIA linac



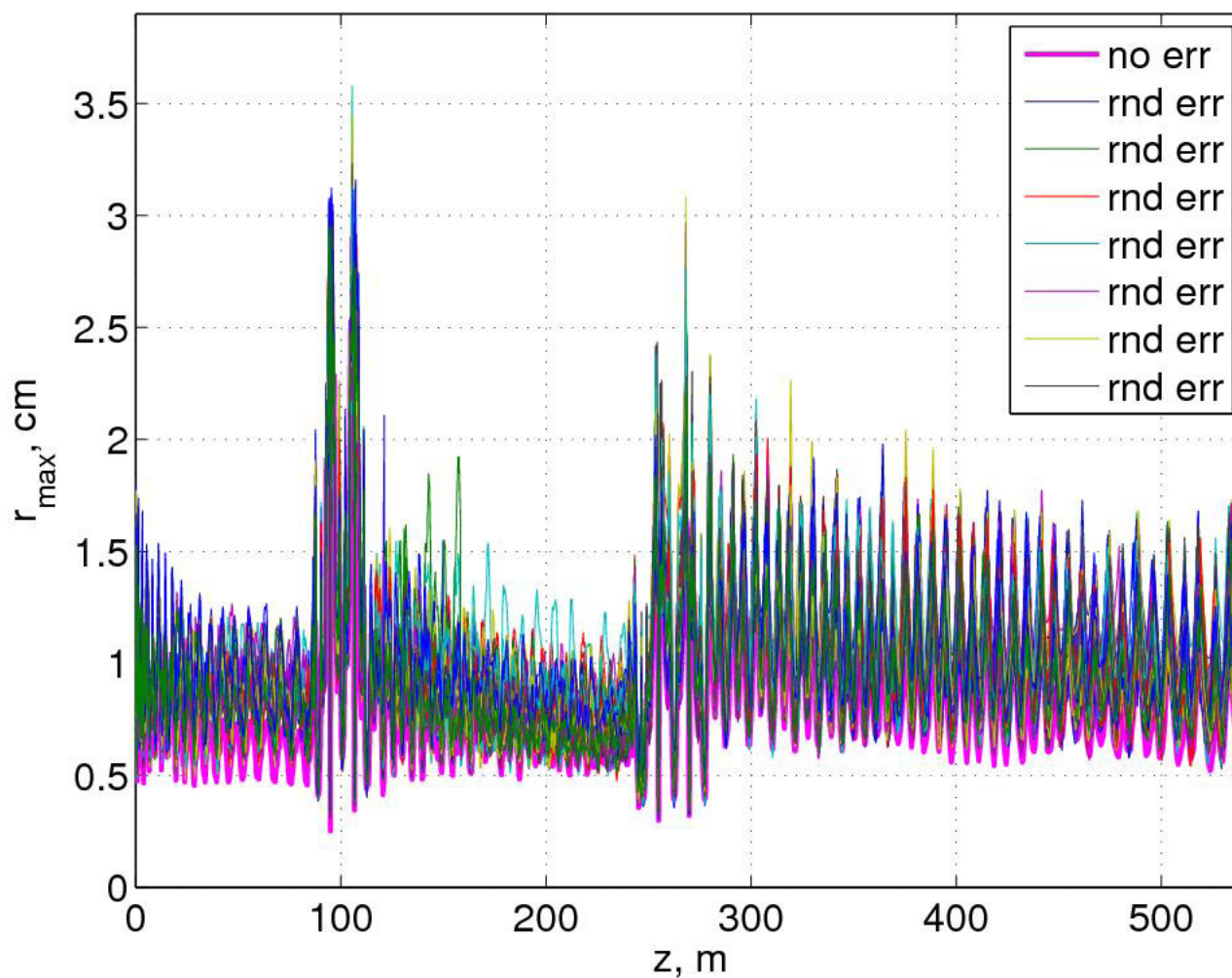
# Beam Centroid and Particle Survive w/o Steering



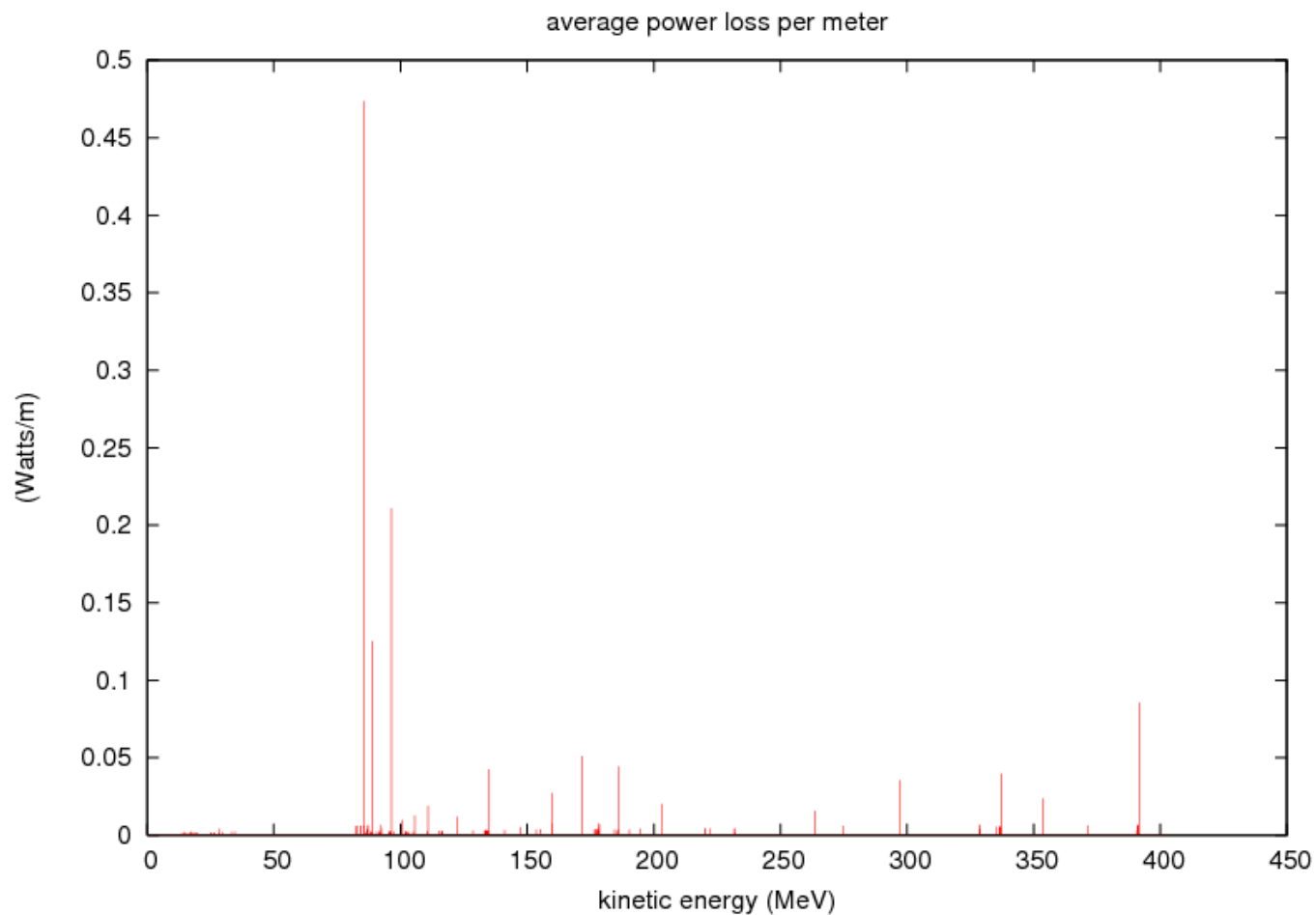
# Horizontal/Vertical Emittance with 100 Random Machine Errors



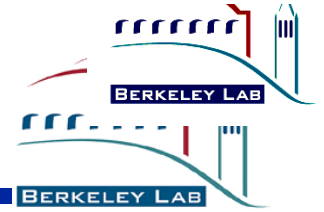
# Maximum Radius Evolution with 100 Random Machine Errors



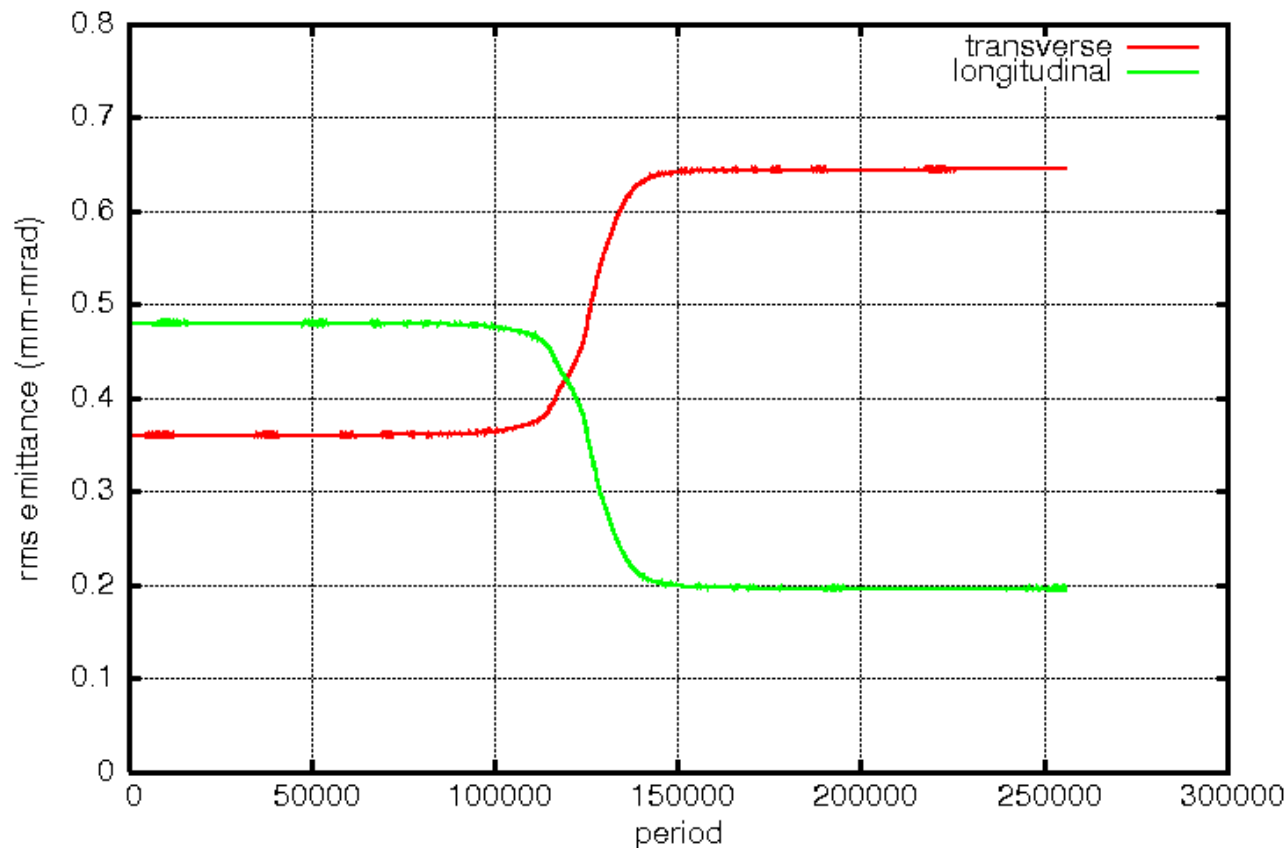
# Average Power Loss Per Meter vs. Kinetic Energy



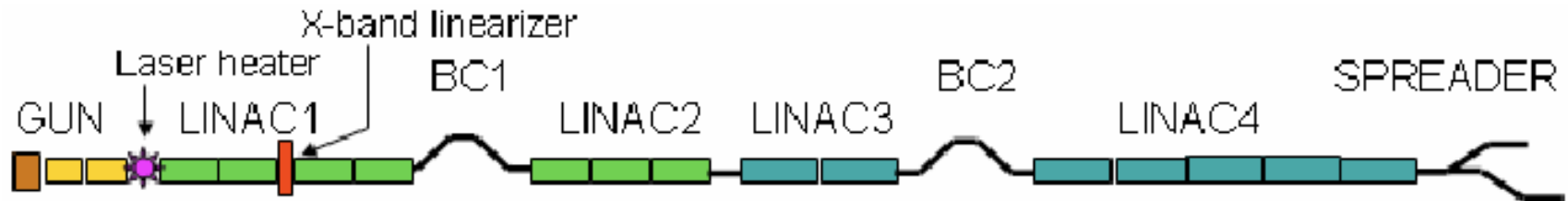
# Long-Term Simulation of Space-Charge Driven Dynamic Emittance Exchange



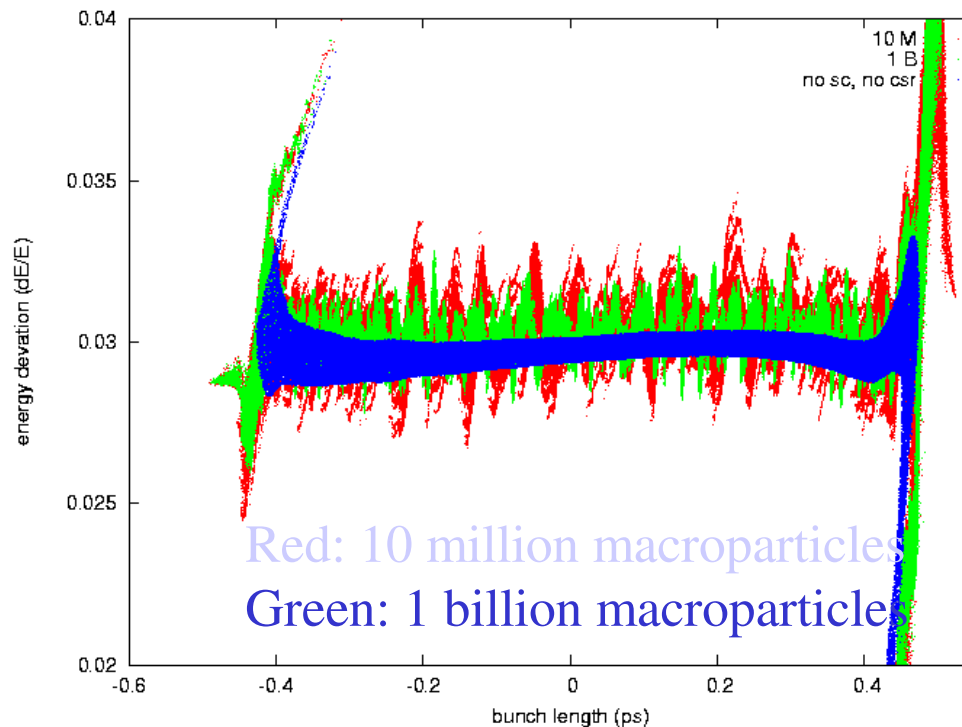
- Not large scale, but time-to-solution unacceptable w/out parallel computing
- IMPACT-Z simulation used 1.3 million space-charge kicks, 32 hrs on 64 procs of IBM/SP5



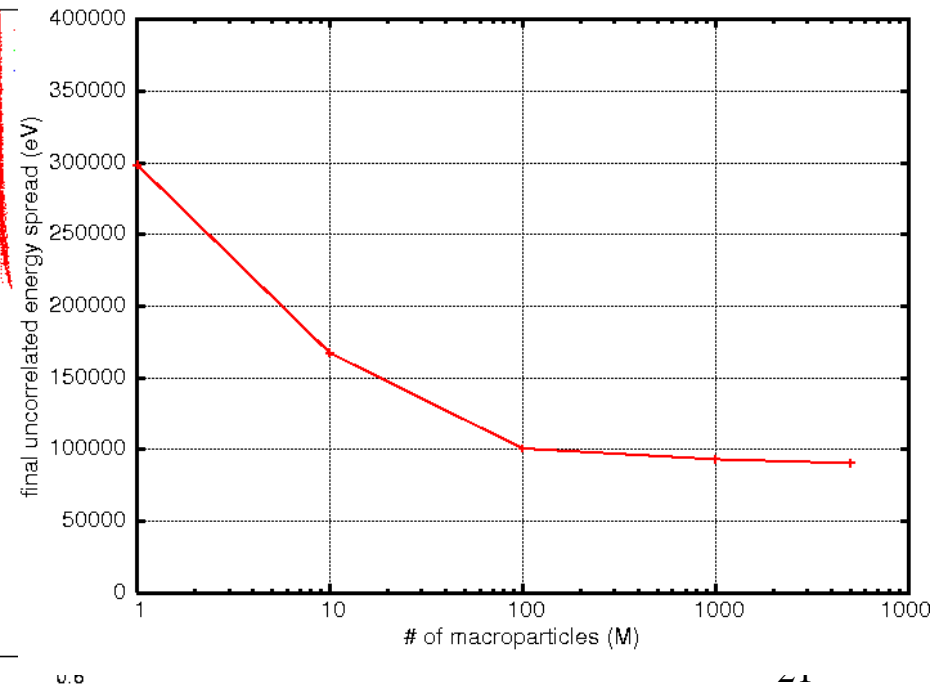
# Future light source design: very large scale modeling of the microbunching instability



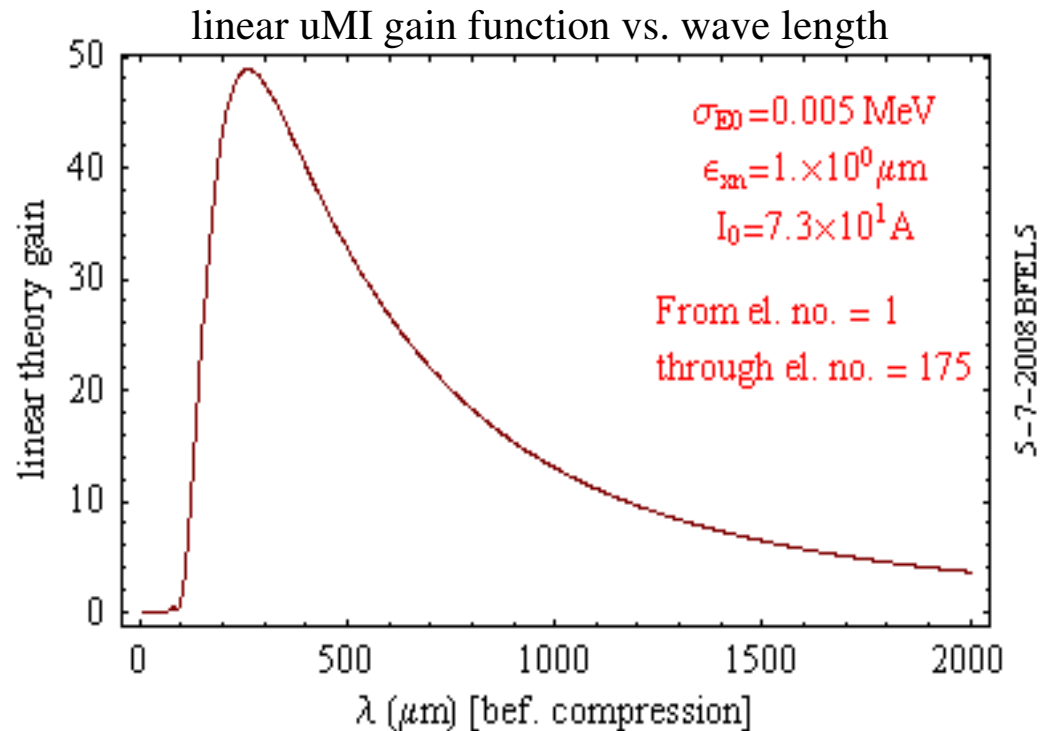
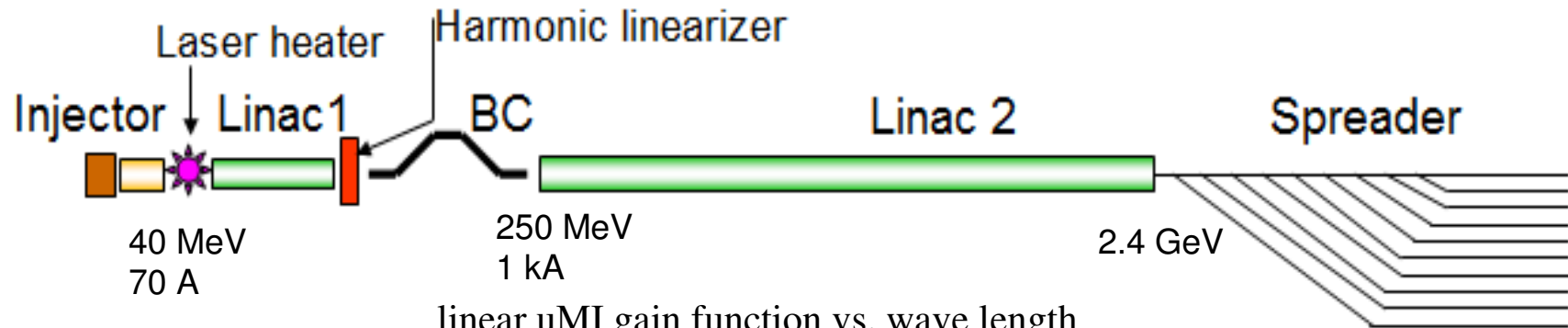
IMPACT-Z simulation showing final longitudinal phase space using 10M and 1B macroparticles



Final Uncorrelated Energy Spread vs. # of Particles



# Beam Delivery System of Berkeley FELs

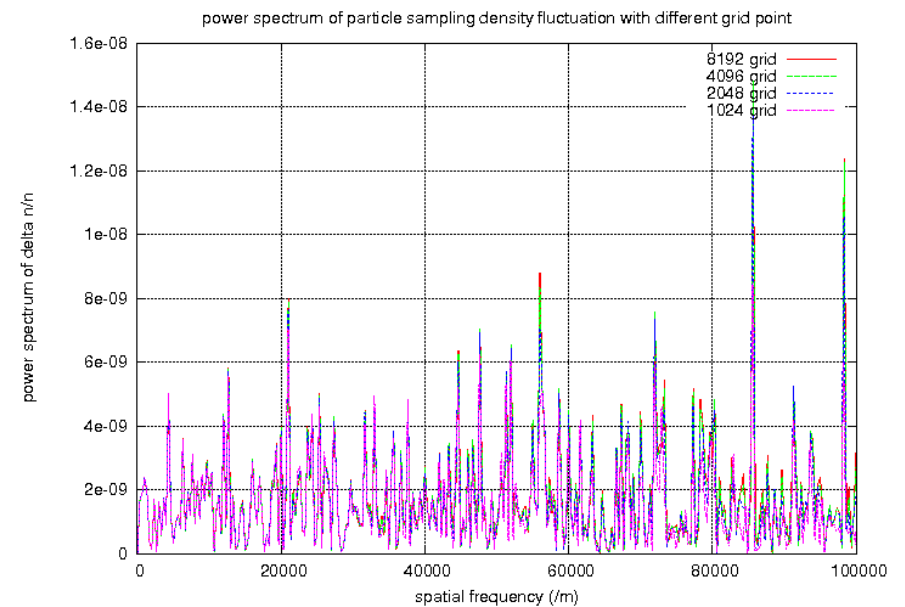
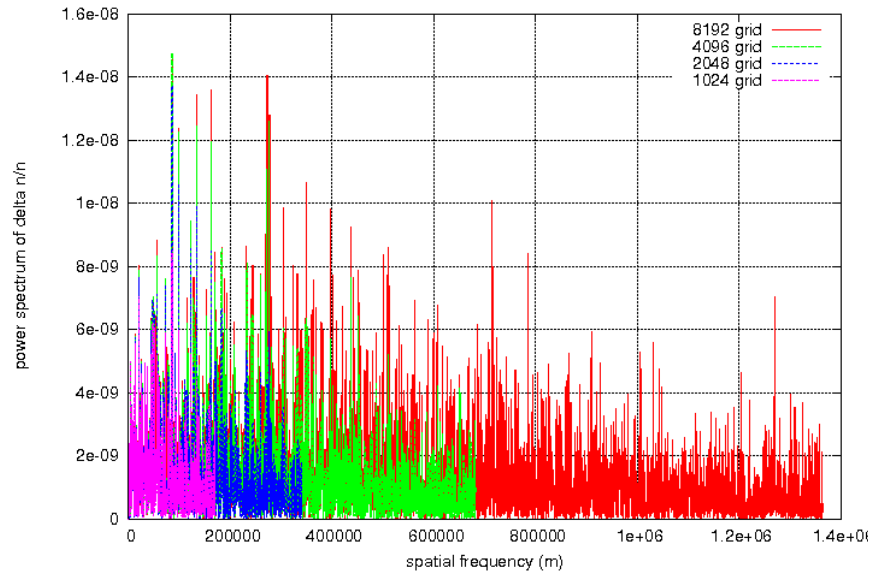


Courtesy of A. A. Zholents and M. Venturini

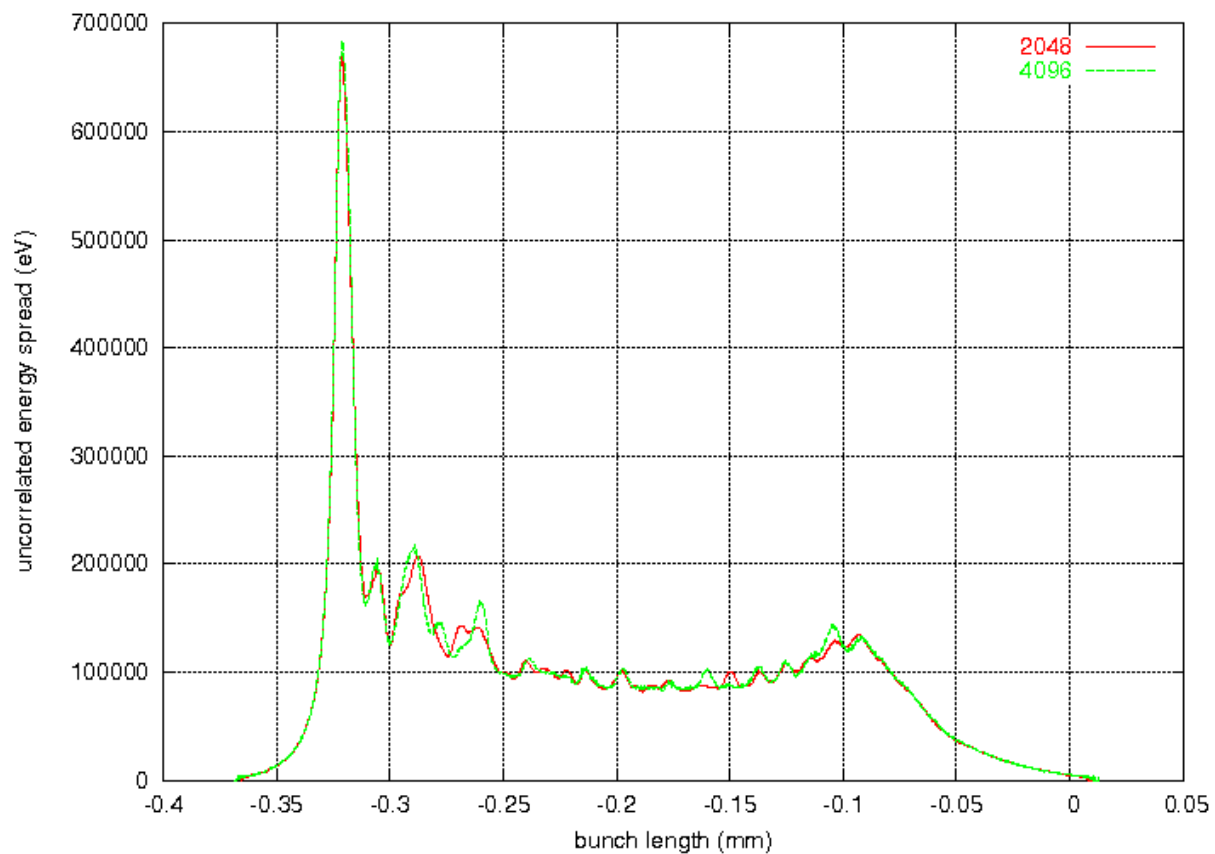
# Choice of Numerical Grid Point



power spectrum of density fluctuation with different grid points



# Final Uncorrelated Energy Spread with Different Number of Grid



# Up Sampling of Initial Particle Distribution

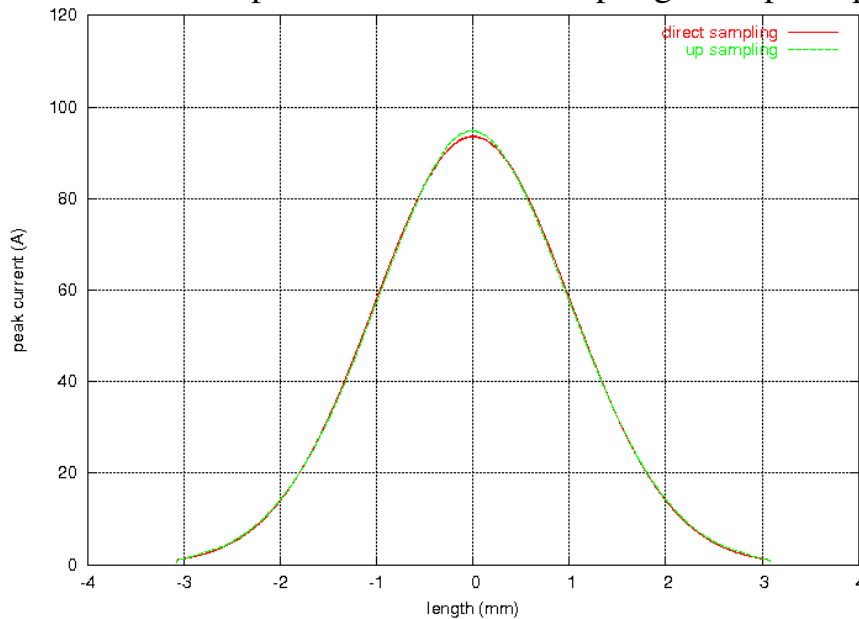


- Maintain global properties of the original distribution
  - emittances
  - current profile,
  - energy-position correlation
- Reduce shot noise of the original particle distribution by using more macroparticles
- A 6D box centered at the original is used to generate new macroparticles
- Uniform sampling in transverse 4D
- Linear sampling in longitudinal position following original current profile
- Cubic spline to obtain the energy-position correlation

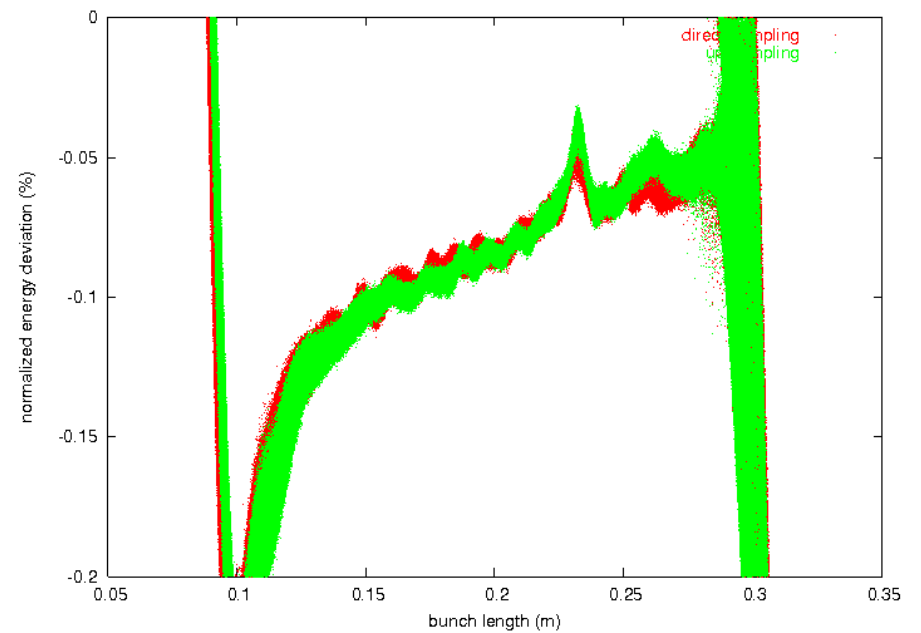
# A Comparison of Direct Sampling and Up Sampling



Initial current profile from direct sampling and up sampling

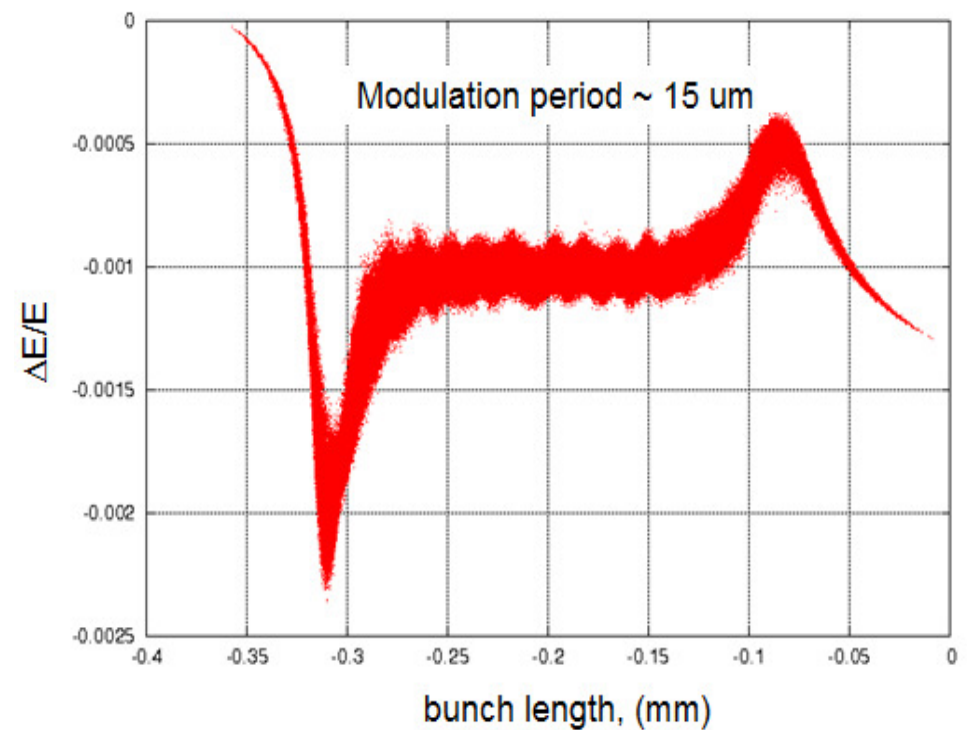
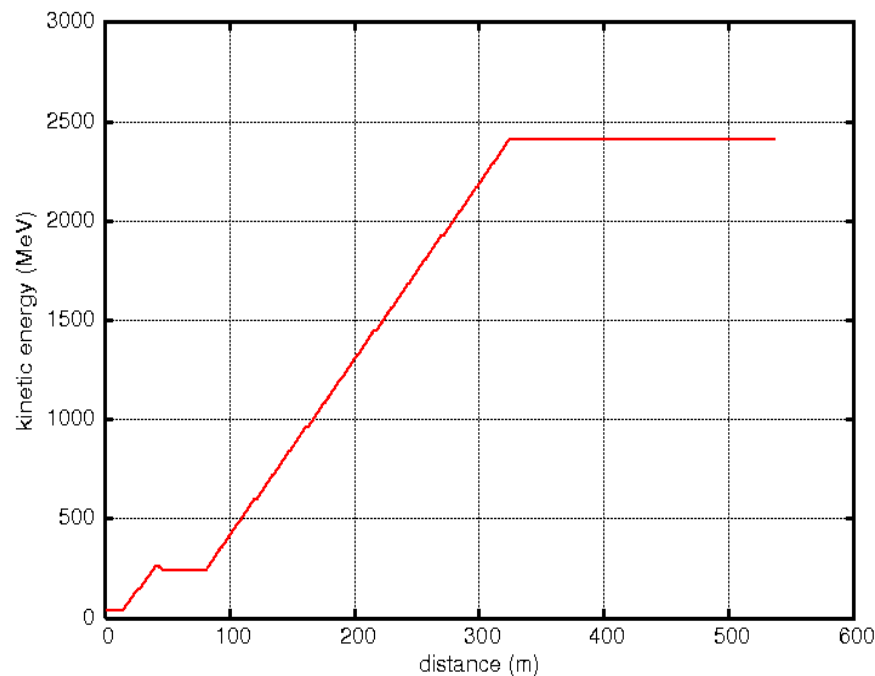
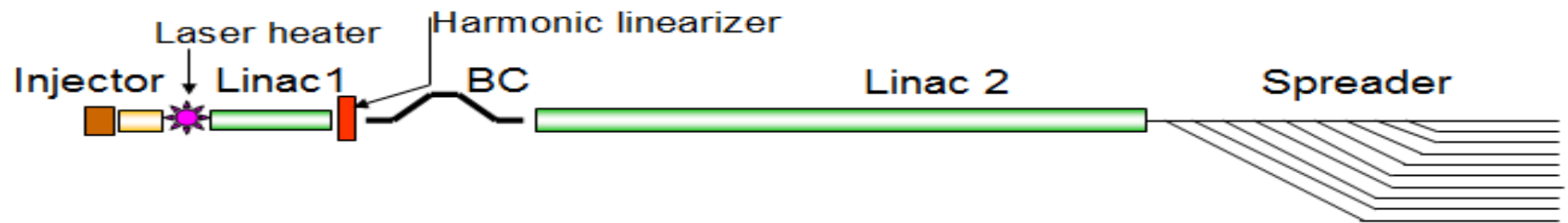


Final longitudinal phase space from direct sampling and up sampling



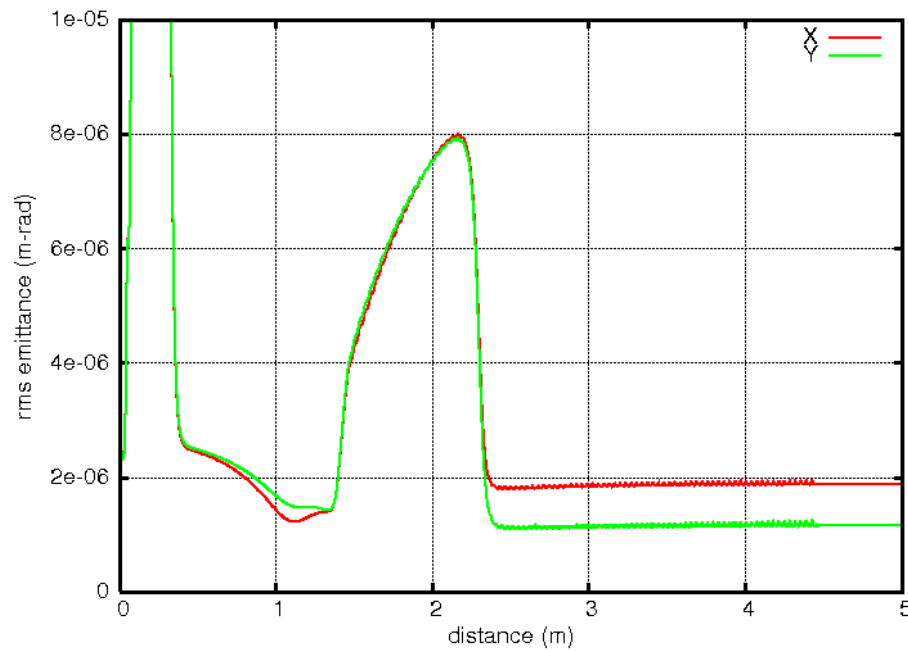
# One Billion Macroparticle Simulation of an FEL Linac

(0.8 nC, from 40 MeV to 2.4 GeV, ~2 hour computing time on 512 processors)



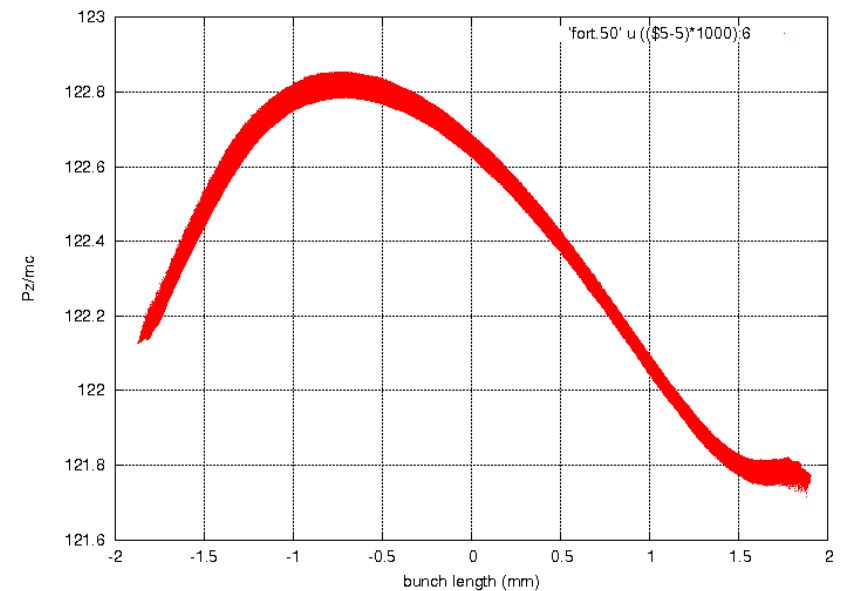
J. Qiang, A. Zholents, LBNL

# Fully 3D Simulation of LCLS Photoinjector



Transverse emittance evolution at LCLS photoinjector with initial 0.5 mm offset

Longitudinal phase space at the end of photoinjector



J. Qiang, LBNL, C. Limbourg, SLAC